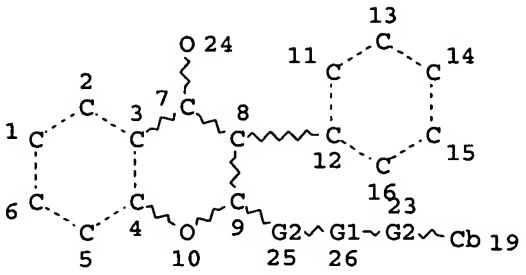


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REP G2=(0-1) CH2
ENTER (DIS), GRA, NOD, BON OR ?:end
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=> s l8
SAMPLE SEARCH INITIATED 09:24:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1319 TO ITERATE

 75.8% PROCESSED    1000 ITERATIONS                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        24202 TO    28558
PROJECTED ANSWERS:               0 TO        0

L9            0 SEA SSS SAM L8

=> s l8 ful
FULL SEARCH INITIATED 09:24:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  25761 TO ITERATE

100.0% PROCESSED   25761 ITERATIONS                             33 ANSWERS
SEARCH TIME: 00.00.01

L10           33 SEA SSS FUL L8

=> s l10 not l7
L11           5 L10 NOT L7

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
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FULL ESTIMATED COST                               312.10     480.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -2.21

FILE 'CAPLUS' ENTERED AT 09:24:27 ON 28 JUL 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 28 Jul 2004 VOL 141 ISS 5
FILE LAST UPDATED: 27 Jul 2004 (20040727/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

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=> s l11
L12          5 L11

=> d bib abs hitstr 1-5

L12  ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2004:120686  CAPLUS
DN   140:181248
TI   Preparation of 2-heterosubstituted 3-aryl-4H-1-benzopyran-4-ones as novel
     therapeutics in breast cancer
IN   Brueggemeier, Robert; Kim, Young-Woo
PA   The Ohio State University Research Foundation, USA
SO   PCT Int. Appl., 33 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
PI   WO 2004012682     A2    20040212       WO 2003-US24520  20030804
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
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             GW, ML, MR, NE, SN, TD, TG
     US 2004087586     A1    20040506       US 2003-634463   20030804
PRAI US 2002-400742P   P     20020802
OS   MARPAT 140:181248
GI
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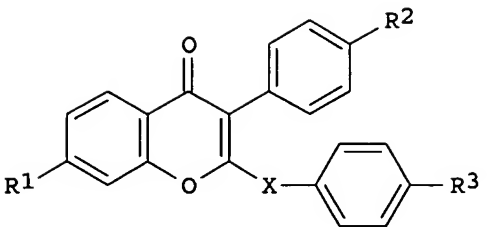

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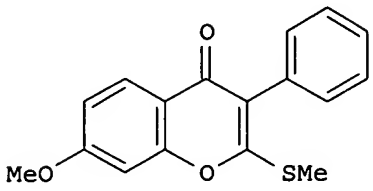


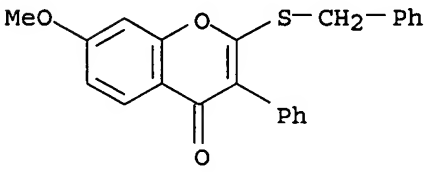
II

AB The present invention provides the title compds. I [X = O, N, S, SO, SO2; R1, R2 = H, OH, OMe, OEt, etc.; R3 = H, OH, OMe, NH2, etc.] for the treatment of cancers, namely breast cancer (biol. data given). This invention further provides a method of synthesis of 2-(alkylthio)isoflavones such as II that can be carried out at ambient conditions. This invention further provides a method of synthesis of the compds. I from a 2-(alkylthio)isoflavone. Thus, a multi-step synthesis of I [X = S; R1 = OH; R2 = OMe; R3 = 2-piperidinoethoxy] which was found to be the most potent in suppressing proliferation of human breast cancer cell lines (IC50 = 0.058 μM), was given. The invention further provides methods of using the compds. I for the treatment of breast cancer in mammals.

IT **474391-06-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-heterosubstituted 3-aryl-4H-1-benzopyran-4-ones as novel therapeutics in breast cancer)

RN 474391-06-5 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-methoxy-3-phenyl-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)



L12 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:586178 CAPLUS

DN 137:352798

TI A convenient one-pot synthesis of 2-(alkylthio)isoflavones from deoxybenzoins using a phase transfer catalyst

AU Kim, Young-Woo; Brueggemeier, Robert W.

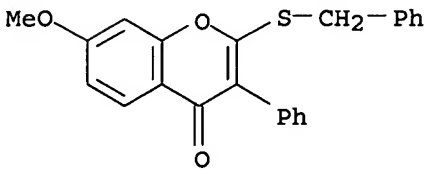
CS College of Pharmacy, Division of Medicinal Chemistry and Pharmacognosy, The Ohio State University, Columbus, OH, 43210-1291, USA

SO Tetrahedron Letters (2002), 43(35), 6113-6115
CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

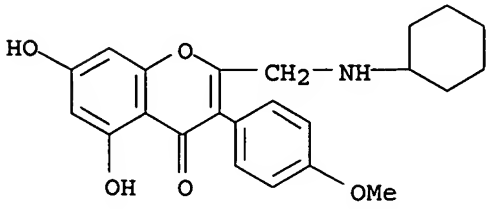
LA English
OS CASREACT 137:352798
AB A convenient phase transfer catalysis procedure for the synthesis of 2-(alkylthio)isoflavones is described. A number of compds. of potential pharmaceutical interest can be prepared in a single step at ambient conditions from various, easily accessible deoxybenzoins using this method.
IT **474391-06-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-pot synthesis of (alkylthio)isoflavones from deoxybenzoins using a phase transfer catalyst)
RN 474391-06-5 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-methoxy-3-phenyl-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)




RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:419930 CAPLUS
DN 111:19930
TI Inhibition of tyrosine protein kinase activity by synthetic isoflavones and flavones
AU Ogawara, Hiroshi; Akiyama, Tetsu; Watanabe, Shunichi; Ito, Noriki; Kobori, Masato; Seoda, Yoshiko
CS Dep. Biochem., Meiji Coll. Pharm., Tokyo, 154, Japan
SO Journal of Antibiotics (1989), 42(2), 340-3
CODEN: JANTAJ; ISSN: 0021-8820
DT Journal
LA English
AB In order to clarify structure-activity relations, the inhibitory activity of flavonoids was investigated against EGF receptor kinase (I). Prunetin, kaempferol, and quercetin exhibited high inhibitory activity. The inhibitory activity was decreased drastically either by the removal of an OH group from the 5-position (flavone and daidzein) or by the addition of a OMe group to the 4'-position (biochanin A and acacetin). The addition of a OMe group at the 7 position (prunetin) also reduced the inhibitory activity. Especially, a bulky group at the 7-position, such as O-glucose (genistin), completely abolished the activity. These results indicated that an OH group at the 5-position is essential for inhibitory activity and that at the 7- and 4'-positions is necessary for full expression of the activity. Although quercetin was highly active against I, it also has previously been shown to inhibit other enzymes, such as cAMP-dependent protein kinase, protein kinase C, phosphorylase kinase, Na+, K+-ATPase, and 5'-nucleotidase. The inhibitory activity of several of the compds. tested, however, was highly specific for I. The cytotoxic effect of isoflavones on RSV3Y1 cells was also examined IC50 values of several compds. tested against the growth of RSV-transformed cells were >100 μg/mL, although they showed a considerably high inhibitory activity against I. Therefore, no close correlation was observed between the inhibitory activity against I and the inhibition of cell proliferation. Similar results were also obtained with flavonoids. All the flavonoids examined exhibited a fair inhibitory activity on the proliferation of RSV3Y1 cells, although some compds., such as daidzein and flavone, showed a poor inhibitory effect on I.

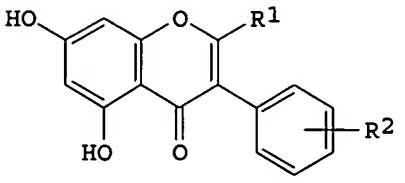
IT **114316-93-7**
RL: BIOL (Biological study)
(EGF receptor kinase inhibition by, structure in relation to)
RN 114316-93-7 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-[(cyclohexylamino)methyl]-5,7-dihydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:204402 CAPLUS
DN 108:204402
TI Preparation of isoflavone derivatives and salts thereof as oncostatic and immunosuppressive agents and pharmaceutical compositions containing them.
IN Ito, Noriki; Ogawara, Hiroshi; Watanabe, Shunichi
PA Yamanouchi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 8702982 | A1 | 19870521 | WO 1986-JP586 | 19861117 |
| | W: KR, US | | | | |
| | RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE | | | | |
| | JP 62201882 | A2 | 19870905 | JP 1986-271518 | 19861114 |
| | EP 245518 | A1 | 19871119 | EP 1986-906932 | 19861117 |
| | R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| | US 4841077 | A | 19890620 | US 1987-93025 | 19870716 |
| | US 4960908 | A | 19901002 | US 1988-261388 | 19881021 |
| PRAI | JP 1985-259603 | | 19851118 | | |
| | WO 1986-JP586 | | 19861117 | | |
| | US 1987-93025 | | 19870716 | | |

OS CASREACT 108:204402
GI



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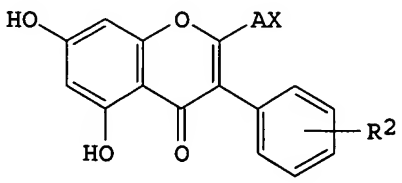

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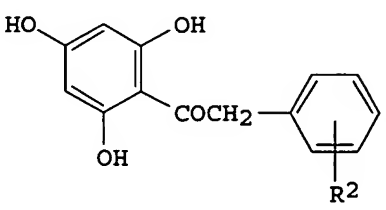


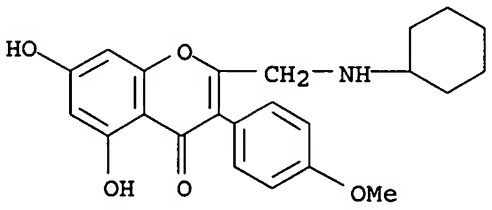
III

AB The title compds. I [R1 = ANR3R4, CONHR5, ASR6, CO2R7 (A = alkylene); R3, R4 = H, (OH-substituted) alkyl, cycloalkyl, 5- or 6-membered heterocyclyl moiety, or NR3R4 may form pyrrolidinyl, piperidinyl, or morpholinyl ring; R5 = H, (OH-substituted) alkyl; R6 = (OH-, CO2H-, or alkoxycarbonyl-substituted) alkyl, S- or N-containing 5- or 6-membered heterocyclyl moiety; R7 = (OH- or alkoxy-substituted) alkyl, when R2 is OH, R7 is C1 or C3-6 alkyl or alkyl substituted with 1 or 2 OH or alkoxy groups; R2 = OH, alkoxy, acyloxy], useful as oncostatic and immunosuppressive agents, were prepared via: (a) reaction of II (A = alkylene; X = halo, organic sulfonic acid residue; R2 = OH, alkoxy, acyloxy) with HNR3R4; (b) amidation of II (AX = CO2H; R2 = as given above) with H2NR5; (c) reaction of II (A = alkylene; X = halo; R2 = as given above) with M1SR6 (M1 = H, alkali metal; R6 = as given above); (d) esterification or transesterification of II (AX = CO2H) or esters/salts thereof using alkanols; and (e) cyclocondensation of acetophenone derivative III with acyl halides. A mixture of acetophenone derivative III (R2 = 4-OH) and ClCOCO2Et in pyridine was stirred for 12 h at 4° to give isoflavone derivative I (R1 = CO2Et, R2 = 4-OCOCO2Et) (IV). IV in vitro exhibited an IC50 of 1 μg/mL against tyrosine specific protein kinase.

IT **114316-93-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as oncostatic and immunosuppressive agent)

RN 114316-93-7 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-[(cyclohexylamino)methyl]-5,7-dihydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)




L12 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1962:475835 CAPLUS

DN 57:75835

OREF 57:15060g-i,15061a-e

TI Synthetic studies on the benzofuran derivatives. VIII. Synthesis of furo[2,3-f]chromeno [3,4-b] chromone

AU Kawase, Yoshiyuki; Numata, Chiji

CS Univ. Toyama

SO Bulletin of the Chemical Society of Japan (1962), 35, 1366-9
CODEN: BCSJA8; ISSN: 0009-2673

DT Journal

LA Unavailable

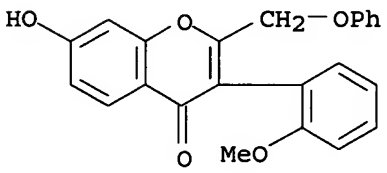
AB cf. CA 57, 2204e. Synthesis of rotenone (CA 56, 1415c) and related products by reduction of chromeno- to chromanochromones indicated the possibility of preparing elliptone (I) from dehydroelliptone (II). The parent nucleus of II, furo [2,3-f]chromeno[3,4-b]chromone (III) was prepared by 2 routes from 7-hydroxy-2'methoxy-2-ethoxymethylisoflavone (IV). In one route, 4 g. IV and 12 g. AlCl3 in 200 cc. benzene was refluxed 2.5 hrs., evaporated, treated with ice H2O and HCl, kept overnight, the precipitate washed with H2O, dissolved in aqueous Na2CO3, filtered, and acidified to give 2',7-dihydroxy-2-hydroxymethylisoflavone (V), m. 225-6° (EtOH)(decomposition), v 3200 (OH), 1630 cm.-1 (γ-pyrone), in 86% yield. A mixture of 2.2 g. V, 22 cc. AcOH, and 33 cc. 50% HBr-AcOH, heated 100° 45 min., and treated with ice H2O gave 2',7-dihydroxy-2bromomethylisoflavone (VI), m. 221-4° (EtOH) (decomposition), in 82%

yield. A solution of 0.9 g. VI in 300 cc. Me2CO was refluxed 4 hrs. with 9 g. K2CO3, then 6 hrs. with 9 g. K2CO3, evaporated, the residue dissolved in H2O, filtered, and acidified to give 9-hydroxychromeno[3,4-b]chromone (VIII), m. 245-50° (EtOH), in quant. yield, 270 λ and 297 mμ (log ε 5.02 and 4.55). A mixture of 1.5 g. VII, 8 g. hexamine, and 60 cc. AcOH was heated on a steam bath 6 hrs. and 10 min. with addition of 27 cc. hot 20% aqueous HCl to give 9-hydroxy-8-formylchromeno[3,4-b]chromone (VIII) as yellowish crystals, m. 261-2° (AcOEt), in 40% yield, v 1730 (CHO) and 1630 cm.-1 (γ-pyrone). A solution of 0.9 g. VIII and 1.2 g. Et bromomalonate in 130 cc. Me2CO was refluxed 8.5 hrs. with 4 g. K2CO3, and evaporated to give ethylfuro [2,3-f]chromeno [3,4-b]chromone-2-carboxylate (IX) as brownish crystals, m. 225-6°, in 36% yield. Saponification of 0.4 g. IX in 30 cc. 5% aqueous NaOH and 115 cc. Me2CO, and acidification with HCl gave the corresponding acid (X) as orange crystals, m. 300° (EtOH) (decomposition), in 68% yield, v 3500, 3320, 1700 (COOH), and 1630 cm.-1 (γ-pyrone). A mixture of 0.2 g. X, 0.1 g. Cu, and 10 cc. quinoline was heated at 190-210° for 20 min. under N, filtered, and steam-distilled to give III as reddish crystals (EtOH, then AcOEt), m. 239.5-40°, in 70% yield. In another route, a solution of 0.4 g. 2' methoxy-2ethoxymethylfuro[2,3-f]isoflavone (XI) (prepared from IV by the method of Matsumoto, et al., CA 53, 16123i) in 30 cc. PhNO2 was treated with 1.2 g. AlCl3 on a steam bath 1 hr., acidified with dilute HCl, steam-distal., extracted with AcOEt, washed dilute HCl, extracted with 5% aqueous NaOH, and acidified with HCl to give 2'-hydroxy-2-hydroxymethylfuro[2,3-f]isoflavone (XII), m. 224-5° (EtOH), in 50% yield, v 3280 (OH), and 1630 cm.-1 (γ-pyrone). A solution of 0.12 g. XII in 40 cc. Me2CO was refluxed with 1.2 g. K2CO3 4 hrs., then 4 hrs. with addition of 1.2 g. K2CO3, filtered, evaporated, and acidified with dilute HCl to give III as slightly orange crystals, m. 241 42.5°, λ 264 and 304 mμ (log ε 4.93 and 4.48), v 1630 cm.-1 (γ-pyrone).

IT **100410-77-3**, Isoflavone, 7-hydroxy-2'-methoxy-2-(phenoxymethyl)-
**100770-40-9**, Isoflavone, 2',7-dihydroxy-2-(phenoxymethyl)-
(preparation of)

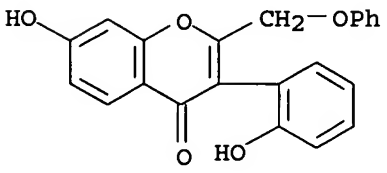
RN 100410-77-3 CAPLUS

CN Isoflavone, 7-hydroxy-2'-methoxy-2-(phenoxymethyl)- (7CI) (CA INDEX NAME)

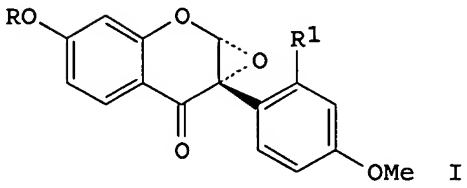



RN 100770-40-9 CAPLUS

CN Isoflavone, 2',7-dihydroxy-2-(phenoxymethyl)- (7CI) (CA INDEX NAME)



AN 1988:131345 CAPLUS
DN 108:131345
TI Acid-catalyzed coupling reactions and conversions of isoflavone epoxides
AU Bezuidenhoudt, Barend C. B.; Brandt, E. Vincent; Ferreira, Daneel
CS Dep. Chem., Univ. Orange Free State, Bloemfontein, 9300, S. Afr.
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (5), 1081-7
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
OS CASREACT 108:131345
GI



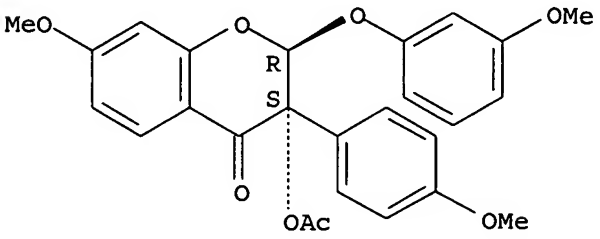
I

AB Whereas isoflavone epoxides I (R = Me, R1 = H; R = tosyl, R1 = tosyloxy) are subject to regioselective acid-mediated methanolysis to yield 2-hydroxy-3-methoxy- and 3-hydroxy-2-methoxy-isoflavones, I (R = CH2Ph, R1 = OCH2Ph) is transformed regiospecifically into the 2-hydroxy-3-methoxyisoflavanone. The course of these coupling reactions is dependent on the benzene ring oxygenation pattern. I (R = Me, R1 = H) reacts with 3-MeOC6H4OH at ambient temperature to give a 3-aryl-2-hydroxyisoflavanone. At 0° the latter compound is accompanied by two regioisomeric O-C-coupled analogs. With phloroglucinol I (R = Me, R1 = H; R = tosyl, R1 = tosyloxy) affords 2,3-diarylbenzofurans which presumably originate via acid-catalyzed conversion of intermediate 3-aryl-2-hydroxyisoflavanones. Differences regarding regioselectively between the nucleophiles (MeOH vs. phenolic compds.), and between the phenolic moieties mutually, are rationalized in terms of the effect of nucleophilicity and of steric constraints imposed on the transition states leading to the resp. regioisomers.

=> d hitstr 3

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
IT **113434-98-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 113434-98-3 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-(acetyloxy)-2,3-dihydro-7-methoxy-2-(3-methoxyphenoxy)-3-(4-methoxyphenyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AN 1998:485049 CAPLUS
DN 129:95354
TI Preparation and formulation of isoflavone derivatives for the prophylaxis and treatment of osteoporosis
IN Chiesi, Paolo; Ventura, Paolo; Servadio, Vittorino; Delcanale, Maurizio; Amari, Gabriele; Armani, Elisabetta; Civelli, Maurizio; Giossi, Massimo; Galbiatti, Elisabetta
PA Chiesi Farmaceutici S.P.A., Italy
SO PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 9829403 | A1 | 19980709 | WO 1998-EP1 | 19980101 |
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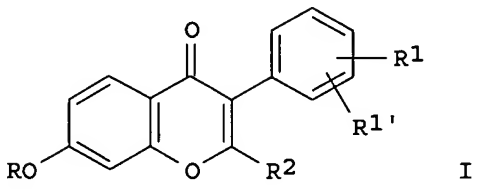
| | RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| | AU 9862066 | A1 | 19980731 | AU 1998-62066 | 19980101 |
| | EP 954520 | A1 | 19991110 | EP 1998-904026 | 19980102 |
| | EP 954520 | B1 | 20020410 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| | AT 215941 | E | 20020415 | AT 1998-904026 | 19980102 |
| | ES 2175661 | T3 | 20021116 | ES 1998-904026 | 19980102 |
| PRAI | IT 1997-MI3 | A | 19970103 | | |
| | WO 1998-EP1 | W | 19980101 | | |

OS MARPAT 129:95354
GI

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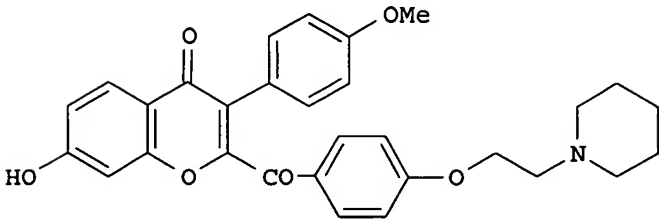



II

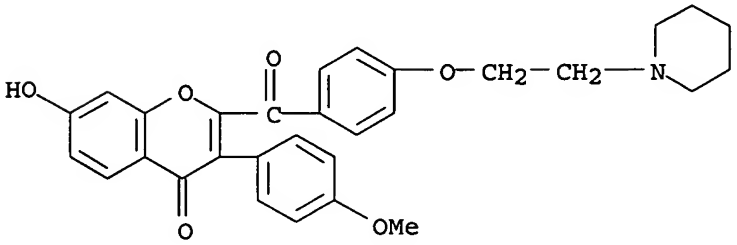
AB Isoflavones I [R = H, alkyl; R1 = H, OH, CF3, OCF3, halogen, alkyl, cycloalkyl, alkoxy; R1' = H, OH, halogen, alkyl, alkoxy; R2 = substituted benzoyl] were prepared for the prophylaxis and treatment of osteoporosis. Thus, isoflavone II.HCl, i.e. CHF 3290.01, was prepared starting from 4-MeOC6H4CH2CO2H, ClCOCO2Et, PhO(CH2)2Br, and piperidine. The prepared

compds. showed good activity in inhibiting bone resorption.

IT **209669-43-2P**, CHF 3290.01 **209669-51-2P**, CHF 3340.01
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and formulation of isoflavone derivs. for the prophylaxis and treatment of osteoporosis)

RN 209669-43-2 CAPLUS

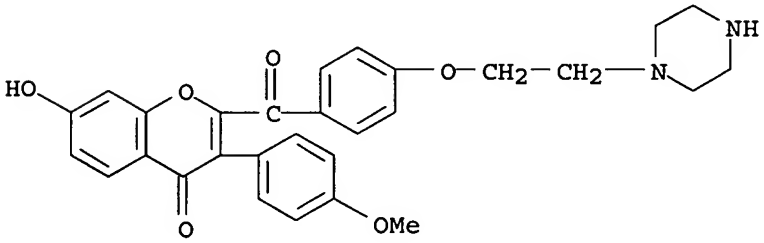
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)-2-[4-[2-(1-piperidinyl)ethoxy]benzoyl]-, hydrochloride (9CI) (CA INDEX NAME)




● HCl

RN 209669-51-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)-2-[4-[2-(1-piperazinyl)ethoxy]benzoyl]-, dihydrochloride (9CI) (CA INDEX NAME)

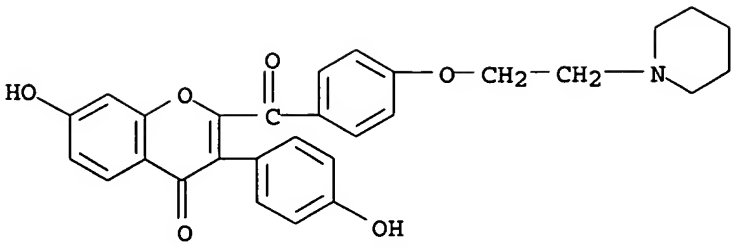



●2 HCl

IT **209669-50-1P**, CHF 3316.01 **209669-52-3P**, CHF 3356.01
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and formulation of isoflavone derivs. for the prophylaxis and treatment of osteoporosis)

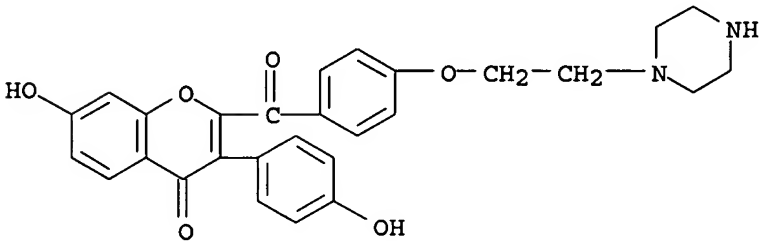
RN 209669-50-1 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[4-[2-(1-piperidinyl)ethoxy]benzoyl]-, hydrochloride (9CI) (CA INDEX NAME)



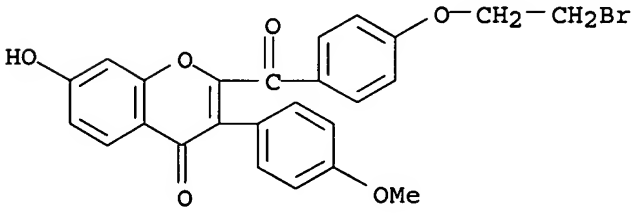
● HCl

RN 209669-52-3 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[4-[2-(1-piperazinyl)ethoxy]benzoyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

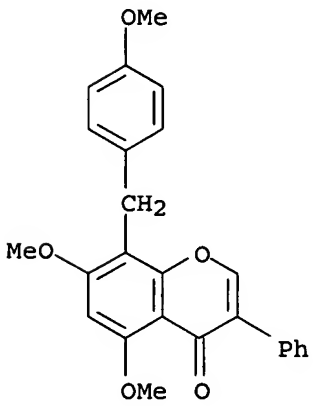
IT **209624-98-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and formulation of isoflavone derivs. for the prophylaxis and treatment of osteoporosis)
RN 209624-98-6 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-[4-(2-bromoethoxy)benzoyl]-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



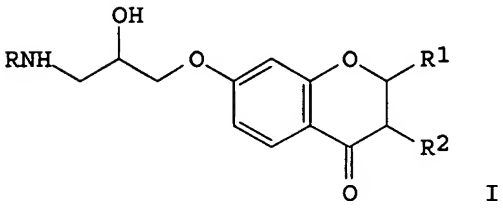
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:645807 CAPLUS
DN 127:314418
TI Anti-invasive activity of alkaloids and polyphenolics in vitro
AU Parmar, Virinder S.; Bracke, Marc E.; Philippe, Jan; Wengel, Jesper; Jain, Subhash C.; Olsen, Carl E.; Bisht, Kirpal S.; Sharma, Nawal K.; Courtens, Andy; Sharma, Sunil K.; Vennekens, Krist'l; Van Marck, Veerle; Singh, Sanjay K.; Kumar, Naresh; Kumar, Ajay; Malhotra, Sanjay; Kumar, Rajesh; Rajwanshi, Vivek K.; Jain, Rajni; Mareel, Marc M.
CS Department of Chemistry, University of Delhi, Delhi, 110 007, India
SO Bioorganic & Medicinal Chemistry (1997), 5(8), 1609-1619
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier
DT Journal
LA English
AB Invasiveness, the ability of certain **tumor** cells to migrate beyond their natural tissue boundaries, often leads to metastasis, and usually dets. the fatal outcome of **cancer**. The need for anti-invasive agents has led the authors to search for possibly active compds. among alkaloids and polyphenolics. One hundred compds. were screened in an assay based on the confrontation of invasive human MCF-7/6 mammary carcinoma cells with fragments of normal embryonic chick heart in vitro. Anti-invasive activity was frequently found among chalcones having a prenyl group. Six compds. were found to inhibit invasion when added to the culture medium at concns. as low as 1 μM. For at least three of them, the anti-invasive effect could be associated with a cytotoxic effect on the MCF-7/6 cells, but not on the heart tissue. This selective cytotoxicity was substantiated by different methods, such as histol. and growth assays (volume measurements, cell counts, MTT and sulforhodamine B assays). The anti-invasive effects of the compds. could neither be ascribed to induction of apoptosis nor to the promotion of cell-cell adhesion. The data indicate that among the alkaloids and polyphenolics, a number of mols. can inhibit growth and invasion of human mammary **cancer** cells via selective cytotoxicity.
IT **116203-33-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(reanti-**tumor** invasive activity of alkaloids and polyphenolics in vitro against human and laboratory animal cells in relation to cardiotoxicity and structure)
RN 116203-33-9 CAPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dimethoxy-8-[(4-methoxyphenyl)methyl]-3-phenyl- (9CI) (CA INDEX NAME)



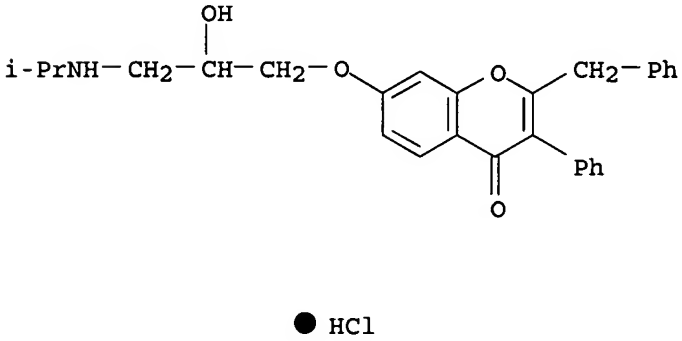
AN 1992:550842 CAPLUS
DN 117:150842
TI Flavones. 3. Synthesis, biological activities, and conformational analysis of isoflavone derivatives and related compounds
AU Wu, Edwin S. C.; Loch, James T., III; Toder, Bruce H.; Borrelli, Alfonso R.; Gawlak, Daniel; Radov, Lesley A.; Gensmantel, Nigel P.
CS Div. Res. Dev., Fisons Pharm., Rochester, NY, 14623, USA
SO Journal of Medicinal Chemistry (1992), 35(19), 3519-25
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI




I

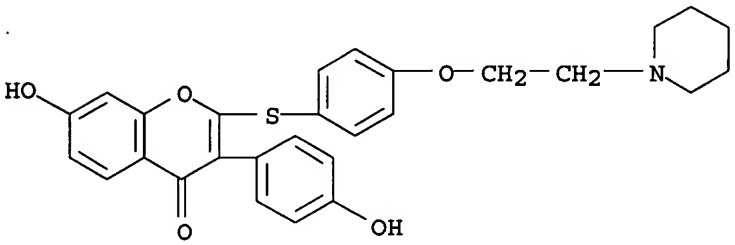
AB A series of 2-alkylisoflavone derivs. I (R = Pr, CHMe2, cyclooctyl; R1 = H, Me, CF3, CHMe2, CH2Ph, 2-furyl, cyclohexyl; R2 = Ph) was prepared in order to study the importance of the Ph group (at the 3-position) of the isoflavone in promoting antihypertensive activity and the substitution effects at the 2-position of isoflavone. With the exception of the 2-iso-Pr analog, the antihypertensive activity of these compds. appears to have a slow onset and long duration. None of the analogs appears better than the corresponding flavone and 3-phenylflavone analogs. An unsuccessful attempt to correlate the relationship between antihypertensive activity and the calculated torsional angle of C2-C3-C1-C2' is discussed. Antiinflammatory activities of these compds. along with 7-(oxypropylamine)flavones were also evaluated and found to be not very potent. The antiinflammatory activity appears to be sensitive to steric effects of the alkyl group on the nitrogen and of substituents at the 2-position of the isoflavones, while the hydroxyl group of the propanolamine side chain is not essential.

IT **143266-84-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antihypertensive and antiinflammatory activity of)
RN 143266-84-6 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-3-phenyl-2-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)

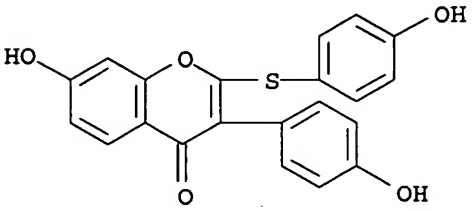



● HCl

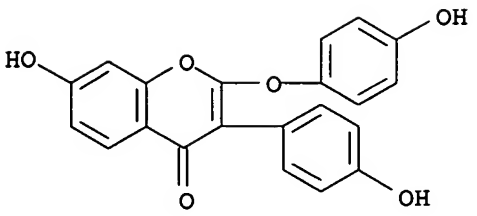
AN 2003:262941 CAPLUS
DN 139:117307
TI Synthesis and estrogen receptor binding affinities of 7-hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-ones containing a basic side chain
AU Kim, Young-Woo; Mobley, James A.; Brueggemeier, Robert W.
CS College of Pharmacy, Division of Medicinal Chemistry and Pharmacognosy, The Ohio State University, Columbus, OH, 43210, USA
SO Bioorganic & Medicinal Chemistry Letters (2003), 13(8), 1475-1478
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 139:117307
AB Two isoflavones containing a sulfur or oxygen hinge with an amine-bearing side chain were designed and synthesized as potential selective estrogen receptor modulators. The target compds. exhibited low affinities for estrogen receptors (ERs), and binding affinity data indicate that oxygen hinge is more favorable than sulfur for binding. These compds. also displayed selectivity for ERα over ERβ.
IT **564476-94-4P 564476-99-9P 564477-01-6P 564477-03-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and estrogen receptor binding affinities of benzopyranone isoflavones containing a basic side chain)
RN 564476-94-4 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[[4-[2-(1-piperidinyl)ethoxy]phenyl]thio]- (9CI) (CA INDEX NAME)



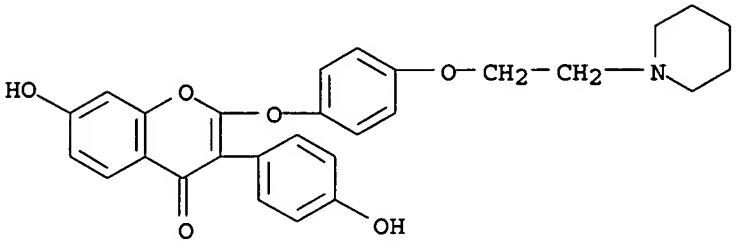

RN 564476-99-9 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)thio]- (9CI) (CA INDEX NAME)




RN 564477-01-6 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-2-(4-hydroxyphenoxy)-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

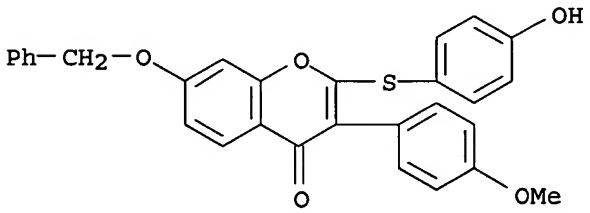


RN 564477-03-8 CAPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[4-[2-(1-piperidinyl)ethoxy]phenoxy]- (9CI) (CA INDEX NAME)

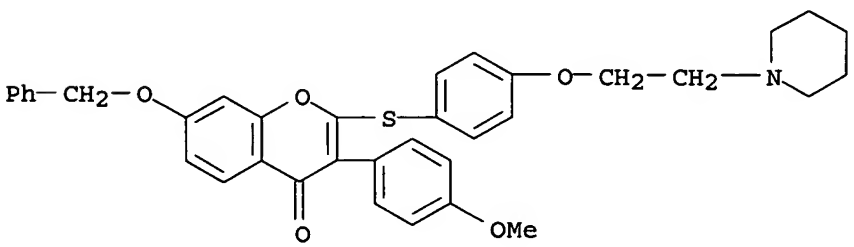


IT **564476-97-7P 564476-98-8P 564477-00-5P 564477-02-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and estrogen receptor binding affinities of benzopyranone isoflavones containing a basic side chain)

RN 564476-97-7 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-[(4-hydroxyphenyl)thio]-3-(4-methoxyphenyl)-7-(phenylmethoxy)- (9CI) (CA INDEX NAME)

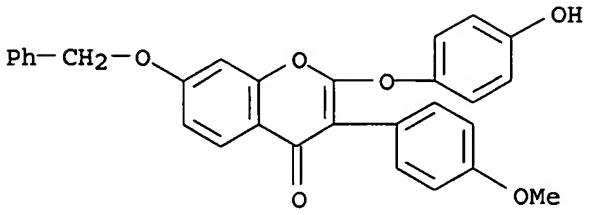


RN 564476-98-8 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-(4-methoxyphenyl)-7-(phenylmethoxy)-2-[[4-[2-(1-piperidinyl)ethoxy]phenyl]thio]- (9CI) (CA INDEX NAME)

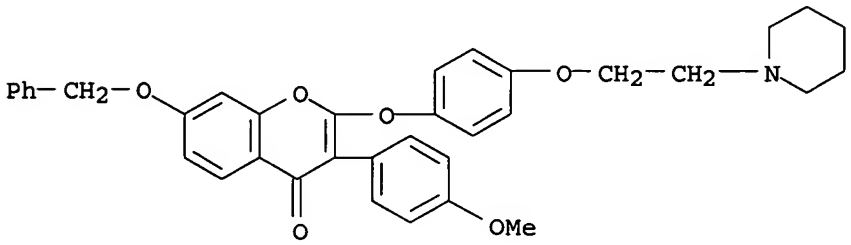


RN 564477-00-5 CAPLUS

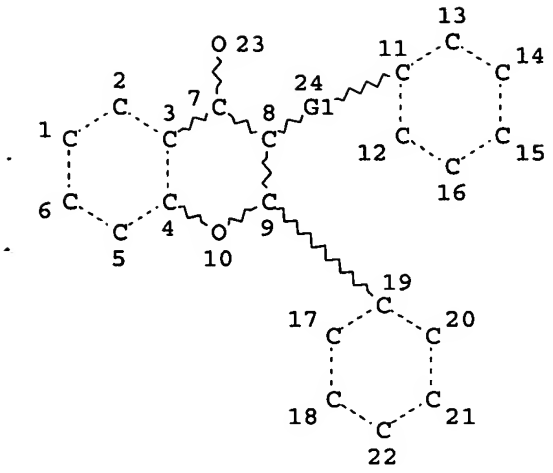
CN 4H-1-Benzopyran-4-one, 2-(4-hydroxyphenoxy)-3-(4-methoxyphenyl)-7-(phenylmethoxy)- (9CI) (CA INDEX NAME)




RN 564477-02-7 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-(4-methoxyphenyl)-7-(phenylmethoxy)-2-[4-[2-(1-piperidinyl)ethoxy]phenoxy]- (9CI) (CA INDEX NAME)




RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT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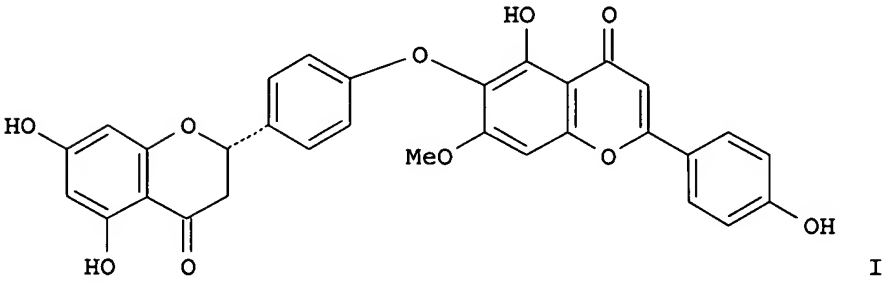
VAR G1=O/S/N/C

AN 2001:243980 CAPLUS
DN 135:31234
TI Three new biflavonoids from selaginella delicatula
AU Lin, Lie-Chwen; Chou, Cheng-Jen
CS National Research Institute of Chinese Medicine, Taipei, 112, Taiwan
SO Chinese Pharmaceutical Journal (Taipei) (2000), 52(4), 211-218
CODEN: CPHJEP; ISSN: 1016-1015
PB Pharmaceutical Society of Republic of China
DT Journal
LA English
GI

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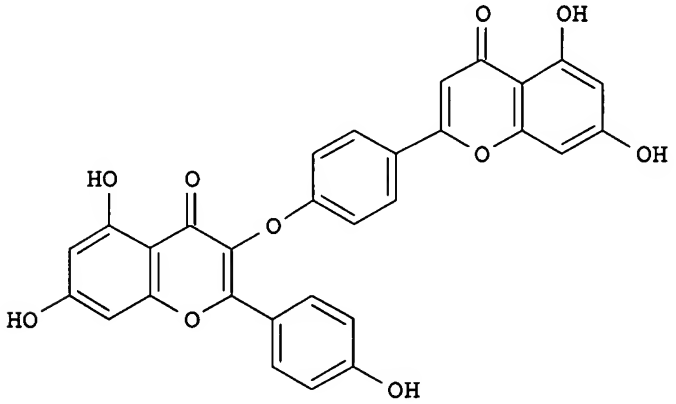



II

AB Three new biflavonoids, 2, 3-dihydroisocryptomerin (I), delicaflavone (II), and 2, 3-dihydrorobustaflavone 7, 4', 7"-trimethyl ether, as well as a known biflavonoid chamaecyparin were isolated from Selaginella delicatula. The structures of these compds. were established by spectroscopic anal. and chemical modification.
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

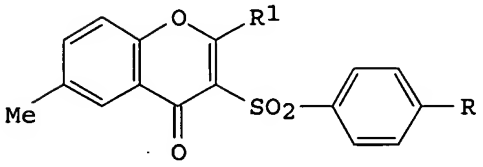
L36 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:228698 CAPLUS
DN 134:261227
TI Anti-mycobacterium flavonoid and chalcone compound compositions and methods of preparing and using them
IN Lin, Yuh-Meej
PA Advanced Life Sciences, Inc., USA
SO PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2001021164 | A2 | 20010329 | WO 2000-US26196 | 20000922 |
| | WO 2001021164 | A3 | 20020110 | | |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | US 6677350 | B1 | 20040113 | US 2000-667131 | 20000921 |
| | EP 1217995 | A2 | 20020703 | EP 2000-963753 | 20000922 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| PRAI | US 1999-155519P | P | 19990922 | | |
| | US 2000-667131 | A2 | 20000921 | | |
| | WO 2000-US26196 | W | 20000922 | | |

OS MARPAT 134:261227

AB The invention provides compds., compns. and methods for the prevention or treatment of mycobacterium infections. The compds. are naturally occurring and synthetic biflavonoids, flavonoids, chalcones and chalcone-like compds. The compds. were screened for anti-mycobacterial activity. Of the compds. showing anti-mycobacterial activity, eight were identified as particularly potent, exhibiting greater than 90% inhibition of the growth of Mycobacterium tuberculosis at a concentration of 12.5 μg/mL. The actual min. inhibitory concns., defined as the lowest concentration inhibiting 99% of the inoculum, for the preferred compds. ranged from 6.8 to 48.3 μM.

AN 1983:522236 CAPLUS
DN 99:122236
TI Synthesis of 2-aryl-3-arylsulfonyl-6-methylchromones as PCA inhibitors
AU Jadhav, K. P.; Ingle, D. B.
CS Dep. Chem., Marathwada Univ., Aurangabad, 431 004, India
SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(2), 150-3
CODEN: IJSBDB; ISSN: 0376-4699
DT Journal
LA English
OS CASREACT 99:122236
GI

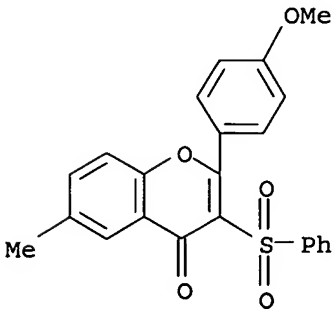


I

AB Condensation of 4-RC6H4SH (R = H, Cl, Br) with 5,2-Me(HO)C6H3COCH2Cl yields 5,2-Me(HO)C6H3COCH2SC6H4R-4 which on oxidation with 30% H2O2 and HOAc give 5,2-Me(HO)C6H3COCH2SO2C6H4R-4. The latter undergo condensation with R1CHO (R1 = Ph, substituted Ph, pyridyl, 2-furyl, 2-thienyl) to form 5,2-Me(HO)C6H3COC(:CHR1)SO2C6H4R-4 which on oxidative cyclization by SeO2 and isoamyl alc. furnish the chromones I. A few compds. are active against passive cutaneous anaphylaxis (PCA) in rats.

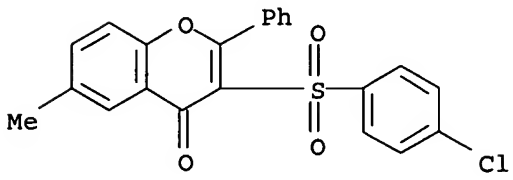
IT **87127-73-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antiallergic activity of)

RN 87127-73-9 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-(4-methoxyphenyl)-6-methyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

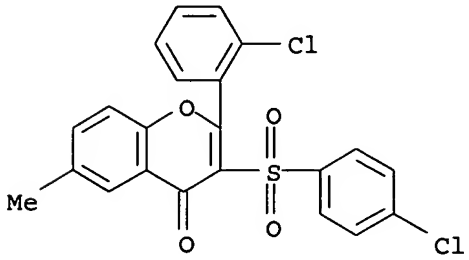



IT **87127-78-4P 87127-79-5P 87127-80-8P**
**87127-81-9P 87127-82-0P 87127-83-1P**
**87127-84-2P 87127-85-3P 87127-90-0P**
**87127-91-1P 87127-92-2P 87127-93-3P**
**87127-94-4P 87127-95-5P 87127-96-6P**
**87127-97-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

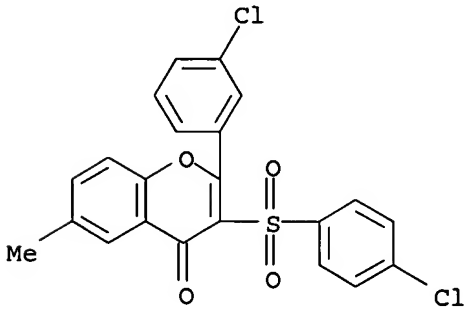
RN 87127-78-4 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-chlorophenyl)sulfonyl]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



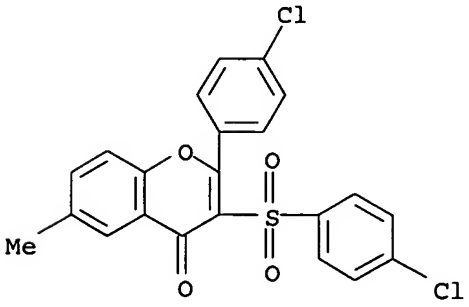

RN 87127-79-5 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-(2-chlorophenyl)-3-[(4-chlorophenyl)sulfonyl]-6-methyl- (9CI) (CA INDEX NAME)



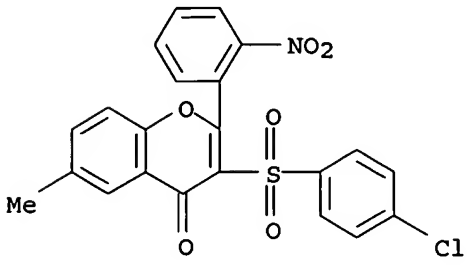

RN 87127-80-8 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-(3-chlorophenyl)-3-[(4-chlorophenyl)sulfonyl]-6-methyl- (9CI) (CA INDEX NAME)



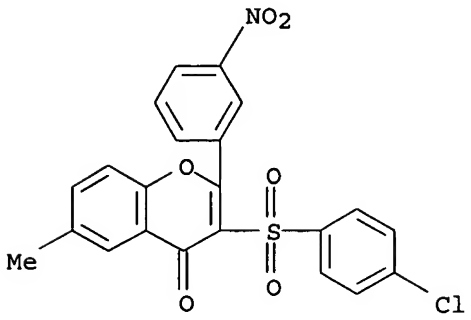

RN 87127-81-9 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-(4-chlorophenyl)-3-[(4-chlorophenyl)sulfonyl]-6-methyl- (9CI) (CA INDEX NAME)



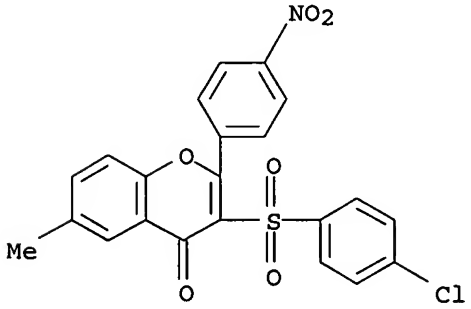
RN 87127-82-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-chlorophenyl)sulfonyl]-6-methyl-2-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



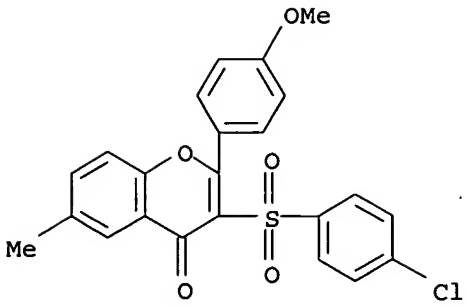

RN 87127-83-1 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-chlorophenyl)sulfonyl]-6-methyl-2-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



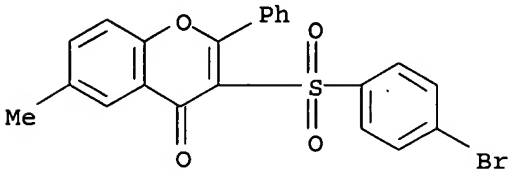

RN 87127-84-2 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-chlorophenyl)sulfonyl]-6-methyl-2-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



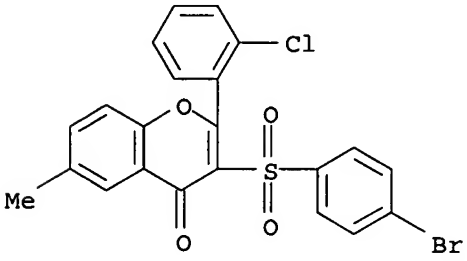

RN 87127-85-3 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-chlorophenyl)sulfonyl]-2-(4-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)



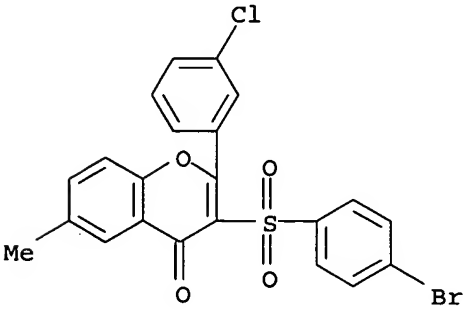

RN 87127-90-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-bromophenyl)sulfonyl]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



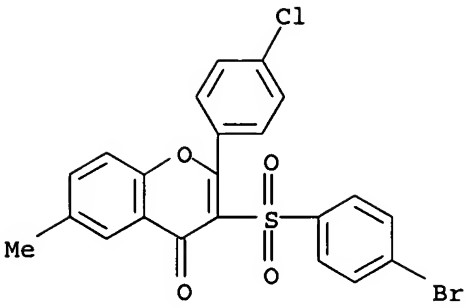

RN 87127-91-1 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-bromophenyl)sulfonyl]-2-(2-chlorophenyl)-6-methyl- (9CI) (CA INDEX NAME)



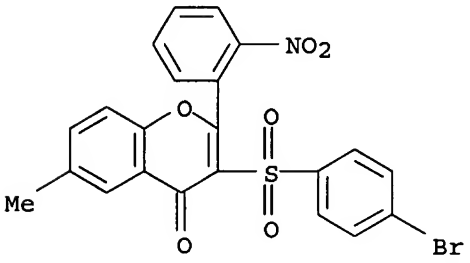

RN 87127-92-2 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-bromophenyl)sulfonyl]-2-(3-chlorophenyl)-6-methyl- (9CI) (CA INDEX NAME)



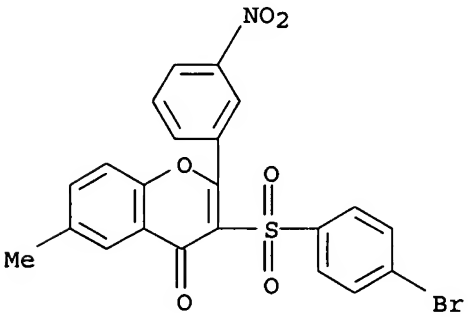

RN 87127-93-3 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-bromophenyl)sulfonyl]-2-(4-chlorophenyl)-6-methyl- (9CI) (CA INDEX NAME)



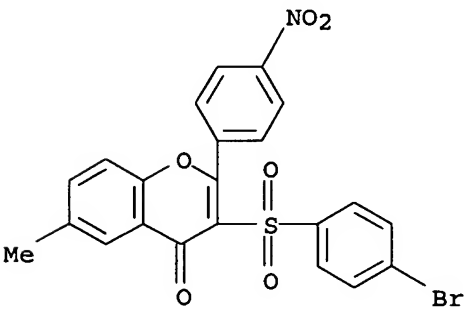

RN 87127-94-4 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-bromophenyl)sulfonyl]-6-methyl-2-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



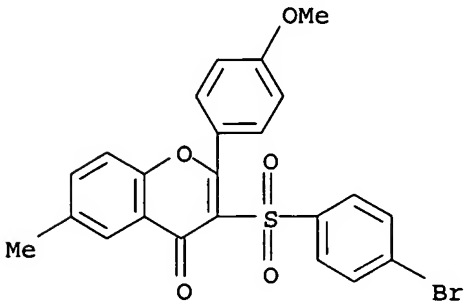

RN 87127-95-5 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-bromophenyl)sulfonyl]-6-methyl-2-(3-nitrophenyl)- (9CI) (CA INDEX NAME)




RN 87127-96-6 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-bromophenyl)sulfonyl]-6-methyl-2-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

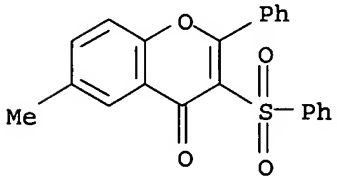


RN 87127-97-7 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[(4-bromophenyl)sulfonyl]-2-(4-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

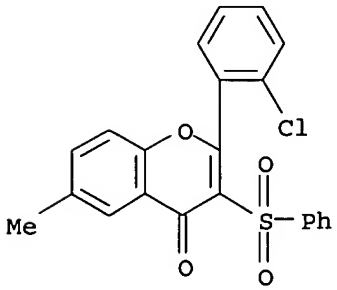



IT **87127-66-0P 87127-67-1P 87127-68-2P**
**87127-69-3P 87127-70-6P 87127-71-7P**
**87127-72-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, cyclization, and antiallergic activity of)

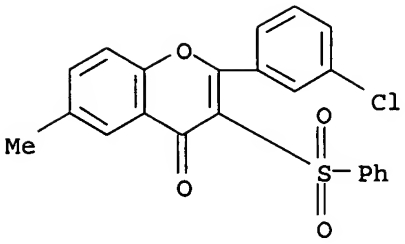
RN 87127-66-0 CAPLUS
CN 4H-1-Benzopyran-4-one, 6-methyl-2-phenyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



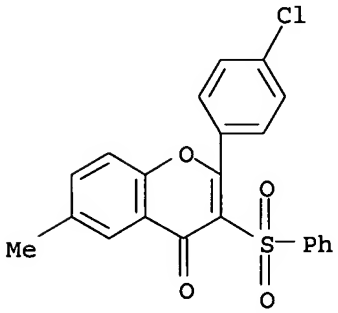

RN 87127-67-1 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-(2-chlorophenyl)-6-methyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



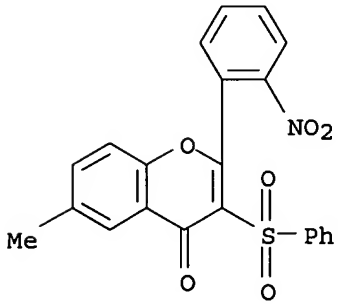

RN 87127-68-2 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-(3-chlorophenyl)-6-methyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



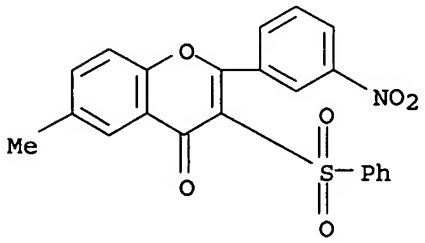
RN 87127-69-3 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-(4-chlorophenyl)-6-methyl-3-(phenylsulfonyl)-
(9CI) (CA INDEX NAME)



RN 87127-70-6 CAPLUS
CN 4H-1-Benzopyran-4-one, 6-methyl-2-(2-nitrophenyl)-3-(phenylsulfonyl)-
(9CI) (CA INDEX NAME)

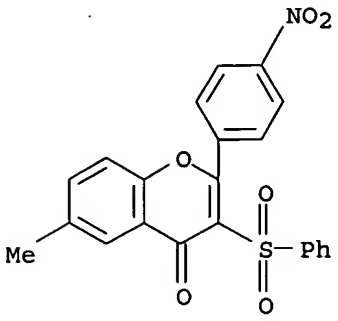


RN 87127-71-7 CAPLUS
CN 4H-1-Benzopyran-4-one, 6-methyl-2-(3-nitrophenyl)-3-(phenylsulfonyl)-
(9CI) (CA INDEX NAME)



RN 87127-72-8 CAPLUS

CN 4H-1-Benzopyran-4-one, 6-methyl-2-(4-nitrophenyl)-3-(phenylsulfonyl)-
(9CI) (CA INDEX NAME)



AN 1996:731856 CAPLUS
DN 126:1217
TI Flavones and coumarins as agents for the treatment of atherosclerosis
IN Saxena, Uday; Trivedi, Bharat Kalidas
PA Warner-Lambert Company, USA
SO PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 9631206 | A2 | 19961010 | WO 1996-US4028 | 19960325 |
| | WO 9631206 | A3 | 19961212 | | |
| | W: AU, BG, CA, CN, CZ, EE, GE, HU, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, UZ, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| | AU 9652592 | A1 | 19961023 | AU 1996-52592 | 19960325 |
| PRAI | US 1995-418709 | | 19950407 | | |
| | WO 1996-US4028 | | 19960325 | | |

OS MARPAT 126:1217

AB Flavones and coumarins or a pharmaceutically acceptable salt thereof are inhibitors of VCAM-1 and ICAM-1 and are thus useful in the treatment of atherosclerosis, restenosis, and immune disorders such as arthritis and transplant rejection. 2-(3-Aminophenyl)-8-methoxychromen-4-one (100 mg/kg) was evaluated in a glucan-induced lung vasculitis in Sprague-Dawley rats and produced 46.2% decrease in monocyte influx and no decrease in neutrophil influx.

IT **5526-51-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(flavones and coumarins for treatment of atherosclerosis, restenosis, and immune disorders)

RN 5526-51-2 CAPLUS
CN 4H-1-Benzopyran-4-one, 3-[[4-(dimethylamino)phenyl]amino]-2-phenyl- (9CI) (CA INDEX NAME)